

Benzenesulfonic acid, 3-hydrazino-
138-30-7 | DTXSID8059681

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.39e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 2.69e-01

Confidence level: 3.05e-01

Nearest Neighbors from the Training Set

Image not found

p,p'-DDE

Measured: 4.46e-11

Predicted: 2.89e-06

Image not found

Naphthalene, 1,2,4,7-tetrachloro-

Measured: 3.45e-10

Predicted: 1.23e-05

Image not found

Phthalic anhydride

Measured: 4.79e-04

Predicted: 9.71e-04

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Dibenzofuran, 1,2,3,4,8-pentachloro-

Measured: 2.84e-11

Predicted: 2.10e-09